IN SEARCH OF THE MISSING LINKS

How multiscale modeling will take engineering to a new level.

BY MIKE VARGO


Amit Acharya

If you looked at a wooden desk only from the scale of atoms and femtoseconds, it would be very dynamic, with everything jiggling around. You wouldn't even know there is something called static equilibrium.

The desk in Amit Acharya's office is a big one, and like most desks it doesn't move: bodies at rest tend to remain at rest, etc. But "this thing is made of atoms," he says, slapping the surface. "If you looked at it only from the scale of atoms and femtoseconds, it would be very dynamic, with everything jiggling around. You wouldn't even know there is something called static equilibrium." Exactly how, then, does Dr. Acharya's desk hang together so solidly? And how hard a blow would make it come apart, and how does that happen?

Such questions lead us into the realm of multiscale modeling, which tries to explain and predict macroscale behavior from events at the microscale. Acharya believes that Carnegie Mellon can be a leader in this emerging field. He is director of CM_2EM, the Center for Multiscale Modeling for Engineering Materials, a new research-and-teaching center that will involve faculty and students from departments throughout CIT and the Mellon College of Science.

The work to be done in CM_2EM is deeply fundamental. We've long had quantum mechanics to explain the atomic world and Newtonian-based theories for the larger scale, but the toolkit is missing some links. There are gaps in our understanding of how micro-phenomena add up to (or influence) larger phenomena, which is often why a semiconductor chip or machine part turns out to have a stubborn flaw – or a new wonder material turns out to have unexpected properties.

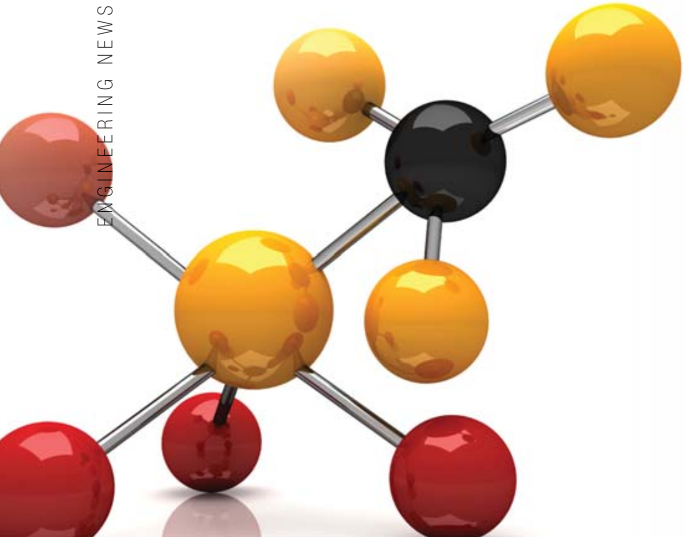
Filling in the gaps is the purpose of multiscale modeling. This work could solve many vexing problems and help us design or alter materials in a more "targeted" fashion; it is "one of the most important challenges of modern-day science that arises from a desire to solve very practical problems," says Acharya, a professor of Civil and Environmental Engineering and Materials Science and Engineering.

Chips, Earthquakes and Super-metals

Some areas where multiscale modeling could pay dividends:

- Thin-film semiconductors and MEMS devices: Chips with ultrathin layers or tiny moving parts are easily spoiled by little strains and cracks – which, in turn, stem from even tinier-scale effects in ways that we don't fully understand or know how to control.
- Earthquake analysis: As Acharya puts it, an earthquake is a very large example of a "stick-and-slip" event, wherein a region of material holds shape for a while and then suddenly gives. Modeling from the fine-grained scale upward can help to predict the give, and though it's unlikely we could ever predict the times and places of earthquakes, even with weather-forecast precision, just doing a better job of it would help us take precautionary steps.
- Amorphous metals: Also called metallic glasses, these alloys are much stronger and springier than equivalent standard metals such as steel, titanium or aluminum. You can buy golf clubs or tennis racquets made with amorphous metals and they are finding their way into other products. Yet many potential uses (notably, in critical structures like airframes) remain beyond reach, because the same quality that makes the new alloys desirable in some respects makes them undesirable or unpredictable in others: their microstructures are different from standard metals.

Amorphous metals have no crystal structure. Their atoms are packed, well, amorphously, as in glass or plastics. This gives them nifty properties like high-yield strengths, since there are no lattice defects to weaken the material, but it raises red flags and unknowns. When these metals do fail they fail



Craig Maloney

oddly – with the formation of "shear bands," tiny parallel cracks that grow and spread – and the important issue of fatigue failure, which can happen from cyclic loading well below the yield strength, is not understood in these materials.

Figuring out why and how this all occurs, and what might be done about it, is a job for multiscale modeling. It is also a job for Craig Maloney.

Getting to the Right Stuff

Craig Maloney is a young first-year faculty member in CEE. With a Ph.D. in physics and postdoc work in materials, he was an unusual hire for a civil and environmental engineering department, but "the recruiting notice specifically said 'multiscale modeling.'" Maloney says he had already made a mark in the field and here was an invitation to do more.

Maloney is running computer simulations of atomic behavior in metallic glasses. He constructs an onscreen grid of one million atoms, applies simulated loads, and watches to see what transpires. This aspect of the work may appear to be pretty much all that there is to multiscale modeling. If we can model a material atom by atom, won't a proper simulation inevitably show the macroscale effects we're interested in, such as how a complete failure mode unfolds from the bottom up?

Alas, it's not that easy. Atoms are so very small and numerous, and the time frames of atomic events are so short, that even high-powered simulations will not take you far up the scale. Maloney's million-atom grid represents only a miniscule slice of a real piece of material. And he has needed runs of "seven or eight hours on a cluster of 128 Athlon computers" just to begin seeing meaningful effects at the atomic scale.

He is looking for simulation results that mathematicians across campus can work with to develop a model of behavior at a scale slightly above the atomic. That would then be tested, and the idea is to keep "bootstrapping" in this manner until the team, ideally, arrives at a true set of "mesoscale" models and theories linking micro-behavior with the macro.

Some shortcuts could speed or simplify the process. For instance, Maloney asks: "At the points where you are shearing the material just enough to get the atoms 'flowing,' can you think of this as similar to a phase transition? [i.e., from solid to liquid or vapor?] If they're analogous, you could borrow a lot of methodology from phase transitions."

But the work is massively complex and massively multidisciplinary. Amit Acharya says Carnegie Mellon has a real advantage in this regard, with its culture of working across disciplines and top talent in every area needed. On a list of some 30 research faculty signed up to participate in CM$_2$EM, Acharya points out names of colleagues: "These guys are world leaders in homogenization, stochastic, and statistical analysis [key techniques from Mathematics and Physics] ... these people [from ChemE and ECE and MechE] are expert experimentalists ... these [from MSE] are the experts in materials ..."

Michael Widom

Michael Widom, a theoretical physicist, is associate director of CM$_2$EM. The center is housed in ICES, the Institute for Complex Engineered Systems. A 'grand-challenge' research thrust for the center is being worked out that will focus on bringing deep scientific analysis to solving a long-standing engineering problem of practical consequence such as, fatigue life of civil infrastructure, aerospace, and MEMS components; stay tuned.

MEET KAUSHIK DAYAL, a new professor and a unique addition to the Civil and Environmental Engineering Department. Dayal's background is in mechanical engineering and aeronautics (his B.Tech. was in naval architecture), and his research at Carnegie Mellon is in materials. It is precisely this broad background that makes Dayal a perfect hire. He explains that the department continues to explore new interdisciplinary research areas important to civil and environmental engineering, such as the research being proposed in the Center for Multiscale Modeling for Engineering Materials (CM$_2$EM).

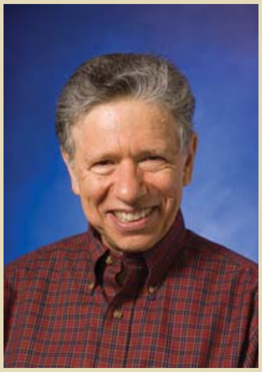
"My goal is to understand and optimize materials, and then I can tell other engineers how to do things in a certain way so we can solve problems," says Dayal, whose present focus is on active or smart materials, used in sensors and actuators. "I look at shape memory. For example, you have a wire and bend it, and then you dip it in hot water, and it gets its shape back." He also works with ferroelectrics, which includes "materials that are used for making electronic memories, like flash drives." Dayal builds his materials on a computer instead of in a lab. "My work involves multiscale modeling of materials," he says.

Just joining Carnegie Mellon in January 2008, Dayal's role in CM$_2$EM will unfold as research projects develop. The center has an education component, and he will teach a graduate course on elasticity this fall. —S.S.

WHEN THE EARTH SHAKES, WHAT WILL REMAIN STANDING?

BY SHERRY STOKES

Understanding how earthquakes behave in large urban areas, like Los Angeles, could save an untold number of lives, but that is not enough, according to Jacobo Bielak of Civil and Environmental Engineering. In earthquake-prone regions, "we also need to prevent the disruption of an area's economy," says Bielak.



Jacobo Bielak

Bielak, who heads a team of researchers from Carnegie Mellon and the University of California, was awarded $1.6 million from the National Science Foundation to develop computer models that will predict how different types of infrastructure will perform during earthquakes.

For more than a decade, Bielak has worked with the Southern California Earthquake Center (SCEC) developing highly evolved models that predict how the ground behaves during an earthquake. "We can do simulations that predict ground motion of a prescribed quake," he says. These models consider, among many things, the magnitude of the quake, its source, the speed and direction it moves along a fault, and the geology of ground basins. Building upon this extensive body of work, Bielak, along with his colleague David O'Hallaron of Electrical and Computer Engineering and Computer Science, intends to expand these models by adding buildings and other infrastructure to the mix. By understanding how groups of buildings react when the ground shakes, people will be better able to prepare for earthquakes and mitigate the damage they may cause.

Populating Models with Buildings

"Typically when analyzing structures for writing building codes, the concentration has been on individual structures," begins Bielak. For years, models have been available that predict how a lone building will hold up during a quake. More recently, earthquake research has yielded powerful models that predict ground motion during a quake for an entire region. For example, Carnegie Mellon researchers have developed a video that shows how a quake that originates on the San Andreas fault can travel and affect nearby communities. Bielak wants to take these ground-motion models, which incorporate the geological features of a region, and populate them with a variety of structures and run simulations. In these new models, an area's geology is extremely important because, as Bielak explains, there can be hot spots within a city where, because of land basins that trap earthquake waves, the earth will shake more.

"We don't want to just learn how individual buildings react," says Bielak. What the researchers want to find out is how a collection of structures that vary in height

and other attributes (i.e., they may have different types of foundations) and are sited on different geological locations (rocky ground versus soft soil) will hold up during earthquakes of varying magnitudes. The same building will respond very differently in different sites within a basin because the ground is moving differently," says Bielak. In addition to buildings, the simulations will include bridges. "In southern California, there are many bridges, and we actually have models of them," says Bielak. (He and others have completed analytical studies on a number of the state's bridges.) Other infrastructure, such as highways, gas lines and pipelines will be examined using the ground deformation as proxy, because, according to Bielak, these structures are very flexible and they tend to follow the ground motion.

> "It is important that we are able to model the ground motion because that allows us to study more naturally how different structures are going to respond to earthquakes."

Where the Research Will Take Us

"Over the last 10 years we have been able to conduct simulations that enable us to predict ground motion," says Bielak. "We can't predict when an earthquake will happen, but we can ask questions. For instance, what if such-and-such earthquake occurs, what will happen?" How will waves radiate away from the quake's starting point? Will the waves become trapped in basins, causing amplification of the ground motion? (Most cities are built on basins.) Which parts of a city are likely to receive the most damage? What types of buildings are likely to remain intact? How can we build and site buildings to sustain the least amount of damage? This last question gives rise to a number of public policy issues.

"Today, if I am going to design a structure that is going to last 100 years, and I want it to withstand earthquakes, I am going to design it so that during the strongest quakes it will suffer some damage, but it should still be functional," explains Bielak. Up until 15 years ago, the goal of earthquake engineers was only to save lives, so a push was on to develop structures that would not collapse, period. "But we need to do better than that," he says, referring to the economic implications of his research.

"If we get a major earthquake every 50 years, do we want to construct a perfect building that costs 300 to 400 percent more to build?" asks Bielak. Erecting these expensive buildings makes sense if they are strategically placed in areas that warrant their construction, but where are these areas? When considering new construction costs and the probability of a major quake occurring, how much damage can an area sustain and remain economically viable? What are the best ways a city can prepare for a quake? "Society must make these decisions," says Bielak. Creating sound public policy is not easy, but Bielak's work will inform decision makers as to what types of structures are best suited for volatile seismic areas.

The images below are from the video titled, "Shake Out," which features a simulation of an earthquake along the San Andreas Fault. CEE graduate students Ricardo Taborda and Leonardo Ramirez, working under their advisor Jacobo Bielak, made the striking video that won the Earthquake Engineering Research Institute's First Annual Graphics Competition in February (http://www.ce.cmu.edu/news/bielak-scec.html)